On the failure of theoretical descriptions of double ionization of helium by high energy electron impact

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It has been stated that the three-body Coulomb problem has been solved numerically, the proof being given through calculations of the single ionization ((e,2e) process) of hydrogen by electron impact [1]. Several numerical recipes like the Convergent-Close-Coupling [2], the Exterior-Complex-Scaling [3], the J-matrrix [4], among others, managed with great success to numerically approach the solution of the problem. A similar success is also obtained when the same methods are applied to the double ionization of helium by photon impact ((γ,2e) process). Except in some minor details, it can be said that the same methods agree remarkably well with each other, and with the experimental observations.

However, for the double ionization of helium by impact of high energy electrons, the (e,3e) process, the same is not observed. In some sense, this brings some doubts on whether the three-body problem can be considered as solved in all cases. On one hand, no method is able to satisfactorily reproduce absolute experimental data [5,6]. On the other hand, the available numerical methods do not yield agreement between each other [7]. When dealing with high energy projectiles the four-body problem corresponding to the (e,3e) process can be reduced to a three-body one. Within such a First Born Approximation, the various numerical methods - which are in such beautiful agreement for (e,2e) and (γ,2e) processes - do not agree with each other when applied to the (e,3e) case.

The aim of this presentation is to pinpoint the reasons behind such a failure, by trying to understand the origin of the disagreement observed between existing numerical methods, to see if they possess intrinsic limitations in applicability or numerical convergence issues, and/or to find out if there exists any additional hidden - not yet understood - difficulty within the Coulomb three-body scattering problem. For this purpose we have proposed two scattering models which should contribute towards this purpose. Both deal with three-body break-up processes, and contain most of the difficulties encountered in real three-body scattering problem, e.g., non-separability in the electrons' spherical coordinates and Coulombic asymptotic behavior.

In Ref. [8,9] we presented a meaningful S–wave model for three particles break–up processes which possesses an analytical solution derived in hyperspherical coordinates; it leads to an analytic expression also for the associated scattering transition amplitude. Since the coordinates' coupling is completely different, the model can be seen as an alternative and complementary test to that given by the Temkin-Poet model [10]. The knowledge of the analytic solution provides an interesting and complete benchmark to test numerical methods dealing with the Coulomb double continuum. The model was used to test an hyperspherical

Sturmian approach recently developed for three–body collisional problems [11,12]. Since the generalized Sturmian basis functions are constructed as to include the correct asymptotic behavior, a very fast convergence of the scattering wave function is observed. The scattering model was also extended to include an hyperangular charge dependence. In that way, one is able to define an approximate S-wave three–body wave function possessing the correct Peterkop behavior at large hyperradii. This extension allowed us to explore the typical structure of the solution of a three-body driven equation, to identify three regions (the driven, the Coulombic and the asymptotic), to quantitatively identify at which hyperradial distances the asymptotic region is really reached, and thus to investigate how far one should go to extract the transition amplitude from the wave function itself.

In a second contribution, the double ionization of helium by high energy electron impact is studied. The corresponding four-body Schrödinger equation is transformed into a set of driven equations containing successive orders in the projectile-target interaction. The transition amplitude obtained from the asymptotic limit of the first order solution is shown to be equivalent to the familiar first Born approximation. The first order driven equation is solved within a generalized Sturmian approach for a S-wave $(e, 3e)$ model process with high incident energy and small momentum transfer corresponding to published measurements. Two independent numerical implementations, one using spherical [13] and the other hyperspherical [11,12] coordinates, yield mutual agreement. From our *ab initio* solution, the transition amplitude is extracted, and single differential cross sections are calculated and could be taken as benchmark values to test other numerical methods in a previously unexplored energy domain.

Both investigations should help in understanding the difficulties associated to the theoretical/numerical description of real high impact energy (e,3e) processes.

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